

University of Groningen

Structure of Escherichia coli lytic transglycosylase MltA with bound chitohexaose - Implications for peptidoglycan binding and cleavage

van Straaten, Karin E.; Barends, Thomas R. M.; Dijkstra, Bauke W.; Thunnissen, Andy-Mark W. H.

Published in:
The Journal of Biological Chemistry

DOI:
[10.1074/jbc.M701818200](https://doi.org/10.1074/jbc.M701818200)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2007

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

van Straaten, K. E., Barends, T. R. M., Dijkstra, B. W., & Thunnissen, A-M. W. H. (2007). Structure of Escherichia coli lytic transglycosylase MltA with bound chitohexaose - Implications for peptidoglycan binding and cleavage. *The Journal of Biological Chemistry*, 282(29), 21197-21205.
<https://doi.org/10.1074/jbc.M701818200>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

SUPPLEMENTARY MATERIAL

STRUCTURE OF *ESCHERICHIA COLI* LYTIC TRANSGLYCOSYLASE MLTA WITH BOUND CHITOHEXAOSE: IMPLICATIONS FOR PEPTIDOGLYCAN BINDING AND CLEAVAGE*

Karin E. van Straaten, Thomas R. M. Barends, Bauke W. Dijkstra and Andy-Mark W. H. Thunnissen

Tables S1 & S2, Figures S1 and S2

Table S1. B-factor analysis and glycosidic linkage conformations in the (GlcNAc)₆-bound sMltA-D308A tetramer

	Average B-factors ^a , Å ²	Average dihedral angles of the β(1,4)-glycosidic linkages ^b	
		Φ, °	Ψ, °
GlcNAc -4	30.8	40.1 (±0.9)	2.2 (±0.4)
GlcNAc -3	25.4	37.5 (±0.7)	-11.0 (±0.7)
GlcNAc -2	25.1	48.4 (±1.0)	7.1 (±1.4)
GlcNAc -1	31.0	-18.4 (±4.4)	-50.3 (±4.2)
GlcNAc +1	39.8	48.1 (±14.2)	-3.0 (±10.8)
GlcNAc +2	52.5		

^aCalculated per subsite and averaged for the equivalent GlcNAc residues in the four bound chitohexaoses.

^bDihedral angles Φ and Ψ are defined by bonds H1_i-C1_i-O4_{i+1}-C4_{i+1} and bonds C1_i-O4_{i+1}-C4_{i+1}-H4_{i+1}, respectively. Values shown are the average values of the equivalent linkages in the four bound chitohexaoses. In brackets are the standard deviations. Favorable (Φ,Ψ) dihedral angles for the glycosidic linkages in chitin and peptidoglycan, as based on molecular dynamic simulations (1) and NMR analysis (2), are (~60°,~0°) and (~68°,~15°), respectively.

Table S2. Residues forming Protein-Sugar Contacts in Chitohexaose-bound sMltA-D308A		
	Van der Waals contacts and hydrogen bonds ^a	Water or phosphate mediated hydrogen bonds
Subsite		
-4	Ser179 (sc,hb); <u>Tyr180</u> (mc); Ala181 (mc); Lys237 (sc)	Lys237; Gln239
-3	<u>Tyr180</u> (mc,sc,hb); Ala247 (sc); Val298 (sc)	<u>Tyr180</u>
-2	Tyr101 (sc); <u>Gly163</u> (mc); <u>Ser164</u> (sc,hb); <u>Tyr180</u> (sc), Lys245 (mc); Gly246 (mc); Ala247 (mc,sc), <u>Asp297</u> (hb), Val298 (sc,mc), Gly300 (mc)	<u>Tyr180</u>
-1	<u>Tyr101</u> (sc), Val161 (mc,sc,hb), <u>Gln162</u> (mc); <u>Gly163</u> (mc); <u>Tyr188</u> (sc); <u>Ala259</u> (sc); <u>Asp297</u> (sc); Val298 (mc); <u>Gly299</u> (mc)	Gly300; <u>Ala301</u>
+1	<u>Gly100</u> (mc,hb); <u>Val161</u> (sc,mc,hb); <u>Gln162</u> (sc,hb); <u>Tyr188</u> (sc); Met208 (sc); <u>Ala301</u> (sc); <u>Ala321</u> (mc); <u>Gly322</u> (mc)	
+2	<u>Thr99</u> (sc), <u>Ser190</u> (sc), Tyr324 (mc), <u>Ala321</u> (mc); <u>Gly322</u> (mc); <u>Asn325</u> (sc,hb),	
^a van der Waals contacts were identified with a 4.0 Å cutoff distance. For hydrogen bonds the acceptor and donor atoms lie between 2.5-3.4 Å apart with favourable geometry. The abbreviations used are: sc, van der Waals contact with side chain; mc, van der Waals contact with main chain; hb, hydrogen bond. Underlined residues are strictly conserved among different MltAs.		

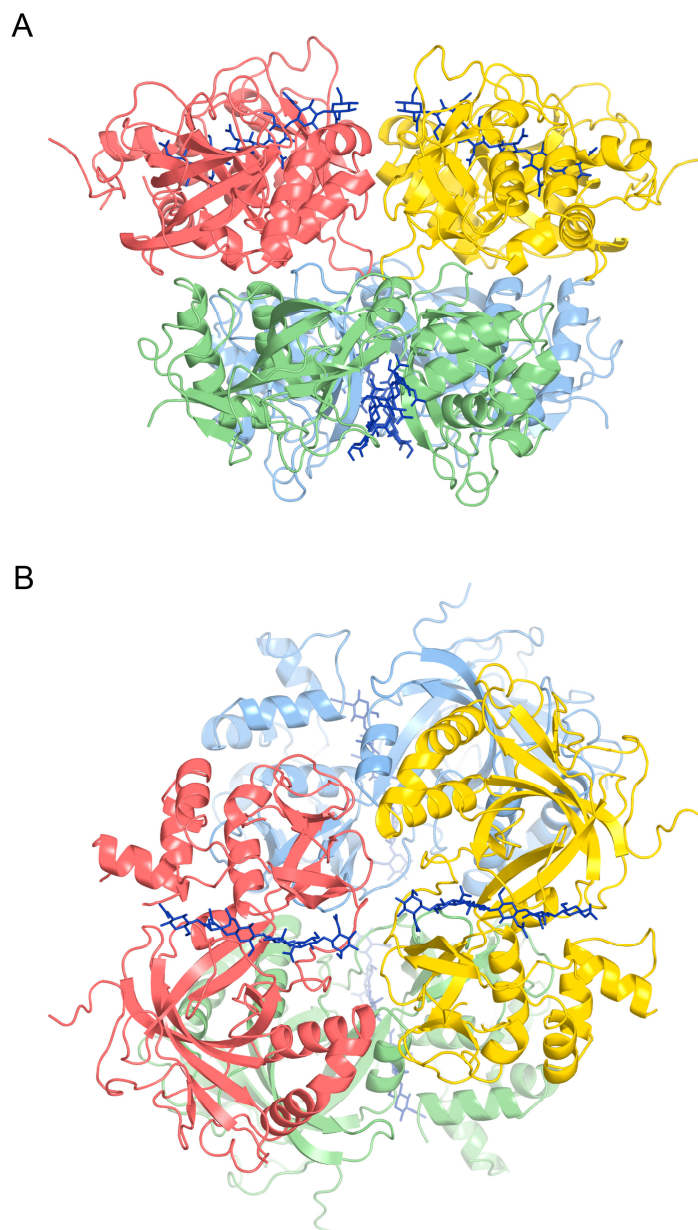


Figure S1. The Crystallographic (GlcNAc)₆-Bound sMltA-D308A Tetramer. *A*, Ribbon representation of the crystallographic (GlcNAc)₆-bound sMltA-D308A tetramer with the sMltA molecules in different colors. The hexasaccharide is shown in blue bonds. *B*, The view in (A) rotated by 90° along the horizontal axis.

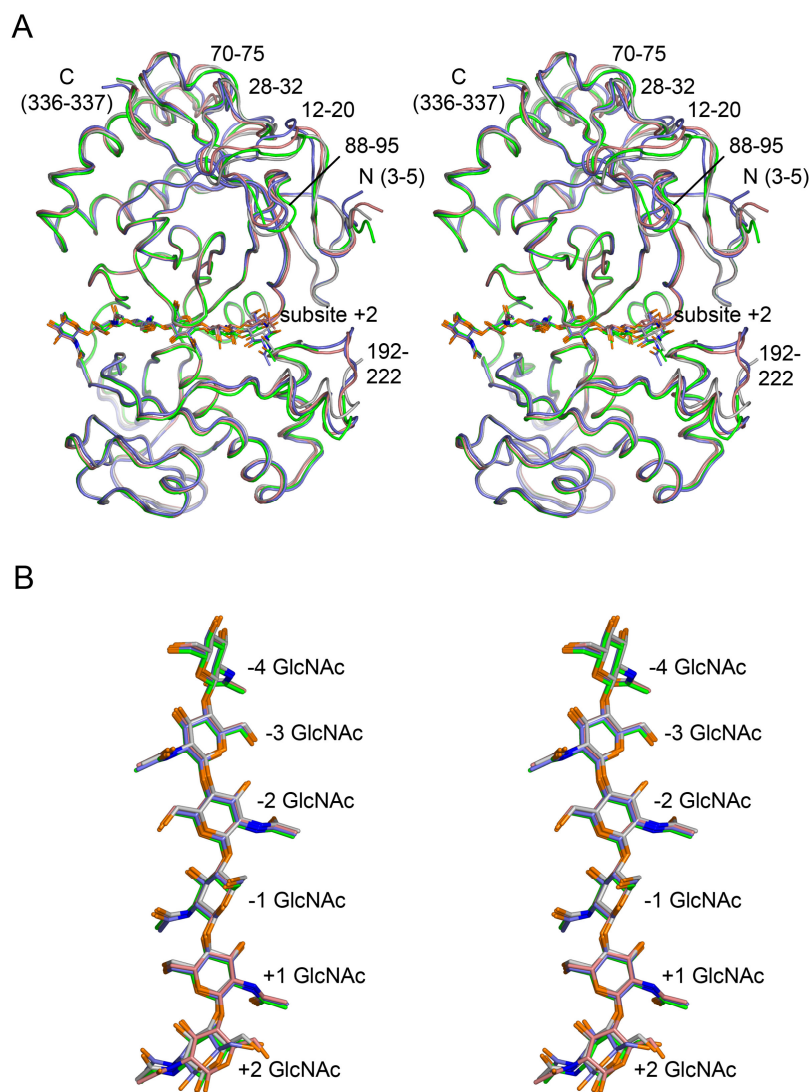


Figure S2. Comparison of the Monomeric Subunit Structures in the Crystallographic (GlcNAc)₆-Bound sMltA-D308A Tetramer. *A*, Stereo view showing a Cα-backbone superposition of the four, differently colored, (GlcNAc)₆-bound sMltA-D308A subunits. Regions in the structures which show substantial differences in conformation are indicated. *B*, Stereo view of an overlay of the four bound (GlcNAc)₆ in the tetramer, obtained by superimposition of the Cα-polypeptide backbones.

References

1. Almond, A., and Sheehan, J.K. (2003) *Glycobiol.* **13**, 255-264.
2. Meroueh, S.O., Bencze, K.Z., Heseck, D., Lee, M., Fisher, J.F., Stemmler, T.L., and Mobashery, S. (2006). *Proc. Natl. Acad. Sci. USA* **103**, 4404-4409.